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Crystal structure of the ternary silicide $Gd_2Re_3Si_5$

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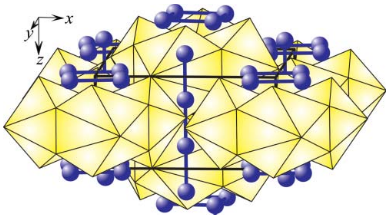
A single crystal of the title compound, the ternary silicide digadolinium trirhenium pentasilicide, $Gd_2Re_3Si_5$, was isolated from an alloy of nominal composition $Gd_{20}Re_{30}Si_{50}$ synthesized by arc melting and investigated by X-ray single-crystal diffraction. Its crystal structure belongs to the $U_2Mn_3Si_5$ structure type. All atoms in the asymmetric lie on special positions. The Gd site has site symmetry *m*..; the two Mn atoms have site symmetries *m*.. and 2.22; the three Si atoms have site symmetries *m*.., ..2 and 4.. . The coordination polyhedra of the Gd atoms have 21 vertices, while those of the Re atoms are cubooctahedra and 13-vertex polyhedra. The Si atoms are arranged as tricapped trigonal prisms, bicapped square antiprisms, or 11-vertex polyhedra. The crystal structure of the title compound is also related to the structure types $CaBe_2Ge_2$ and W_5Si_3. It can be represented as a stacking of Gd-centred polyhedra of composition [$GdSi_9$]. The Re atoms form infinite chains with an Re—Re distance of 2.78163 (5) Å and isolated squares with an Re—Re distance of 2.9683 (6) Å.



1. Chemical context

Four structure types of composition $R_2T_3Si_5$ are known for the systems *R*–*T*–Si (*R* = rare-earth element, *T* = *d*-block element): $U_2Mn_3Si_5$ (Yarmolyuk *et al.*, 1977) (Pearson symbol *tP*40, space group *P*4/*mnc*), $U_2Co_3Si_5$ (Akselrud *et al.*, 1977) (*oI*40, *Ibam*), $Nd_2Os_3Si_5$ (Rizzoli *et al.*, 2004) (*tP*48, *P*4/*mnc*) and $Lu_2Co_3Si_5$ (Chabot & Parthé, 1985) (*mS*40, *C*2/*c*). The structure type $U_2Mn_3Si_5$ has representatives in the systems *R*–Mn–Si (*R* = Y, Gd–Lu), *R*–Re–Si (*R* = Y, La–Nd, Sm, Gd–Tm), *R*–Fe–Si (*R* = Sc, Y, Sm, Gd–Lu), *R*–Ru–Si (*R* = Sm, Er, Lu), whereas the structure type $U_2Co_3Si_5$ has been found in the systems *R*–Ru–Si (*R* = Tb, Er), *R*–Co–Si (*R* = Sc, Y, Ce, Gd–Er), *R*–Rh–Si (*R* = Y, La, Ce, Nd, Sm, Gd–Er), *R*–Ir–Si (*R* = Y, Ce, Tb, Lu), *R*–Ni–Si (*R* = Y, Ce, Nd, Sm, Gd–Tm), *R*–Pt–Si (*R* = Ce, Sm), and *R*–Pd–Si (*R* = Ce, Sm), the structure type $Nd_2Os_3Si_5$ in the systems *R*–Os–Si (*R* = Nd, Eu), and the structure type $Lu_2Co_3Si_5$ in the systems *R*–Co–Si (*R* = Y, Tb, Dy, Lu), *R*–Rh–Si (*R* = Y, Tb, Dy) and *R*–Ni–Si (*R* = Lu) (Villars & Cenzual, 2013).

2. Structural commentary

The existence of the compound $Gd_2Re_3Si_5$ has been reported earlier (Bodak *et al.*, 1978). The unit-cell parameters were determined and the structure type was assigned. A complete investigation of the crystal structure by X-ray single crystal diffraction has now been undertaken. The coordination polyhedra of the Gd atoms have 21 vertexes, whereas those of the Re atoms are cubooctahedra or 13-vertex polyhedra, and the Si atoms tricapped trigonal prisms, bicapped square anti-

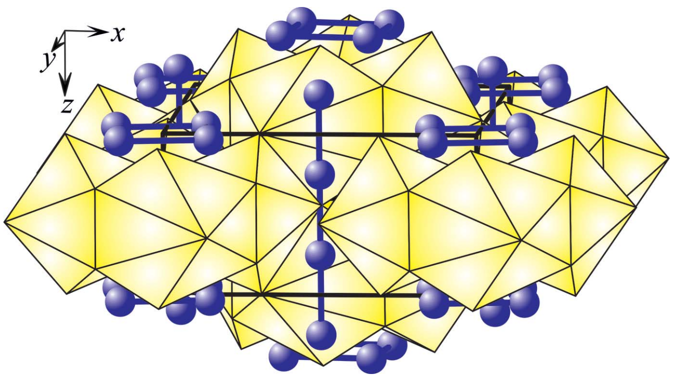


Figure 1
Stacking of Gd-centred polyhedra in the structure of the compound $Gd_2Re_3Si_5$ with displacement ellipsoids drawn at the 99% probability level.

prisms, or 11-vertex polyhedra. The $U_2Mn_3Si_5$-type structure is closely related to the structure type $BaAl_4$ and its ordered derivative $CaBe_2Ge_2$. In particular, the $U_2Mn_3Si_5$-type can be considered to be formed by one-dimensional structural fragments of the structure type $CaBe_2Ge_2$, running parallel to the direction [00l]. There also exists a relationship between the structure types $U_2Mn_3Si_5$ and W_5Si_3. Fragments which can be viewed as deformed square antiprisms are common to both structures. The crystal structure of $Gd_2Re_3Si_5$ can also be represented as a stacking of Gd-centred polyhedra of composition $[GdSi_9]$, located at $z = 0$ and $\frac{1}{2}$ (Fig. 1) (Parthé *et al.*, 1993). The Re atoms form infinite chains with an Re—Re distance of 2.78163 (5) Å and isolated squares with an Re—Re distance of 2.9683 (6) Å.

3. Synthesis and crystallization

An alloy of nominal atom percent composition $Gd_{20}Re_{30}Si_{50}$ was synthesized from the high-purity elements by arc melting on a water-cooled copper plate under a purified argon atmosphere, using titanium as a getter and a tungsten electrode. The weight loss during the sample preparation was less than 0.5% of the total mass (1 g). The alloy was placed into an Al_2O_3 crucible and inserted into a tantalum container, which was then sealed by welding, leaving the sample under an argon atmosphere. The sample, wrapped in tantalum foil, was heated to 1623 K in a muffle furnace at a rate of 200 K h^{-1}, held at this temperature for 5 h and then cooled to room temperature at a rate of 50 K h^{-1}.

4. Refinement details

A single crystal of well-defined shape was separated from the sample. The structure was solved by direct methods. The highest Fourier difference peak of 2.35 e $Å^{-3}$ is at $(0, \frac{1}{2}, \frac{1}{4})$, 0.00 Å away from atom Re2. The deepest hole (−2.44 e $Å^{-3}$) is at (0.6045, 0.3985, 0), 1.52 Å away from the Gd atom. Details of the crystal parameters, data collection and the structure refinement details are summarized in Table 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$Gd_2Re_3Si_5$
M_r	1013.55
Crystal system, space group	Tetragonal, *P4/mnc*
Temperature (K)	293
a, c (Å)	10.95564 (13), 5.56326 (11)
V ($Å^3$)	667.74 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	74.55
Crystal size (mm)	0.16 × 0.10 × 0.02
Data collection	
Diffractometer	Agilent Xcalibur Onyx
Absorption correction	Analytical [*CrysAlis PRO* (Agilent, 2012; analytical numeric absorption correction using a multi-faceted crystal model (Clark & Reid, 1995)]
T_{min}, T_{max}	0.015, 0.194
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11378, 502, 481
R_{int}	0.062
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.692
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.063, 1.17
No. of reflections	502
No. of parameters	31
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	2.35, −2.44

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *WinGX* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

Acknowledgements

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470 Fedyna *et al.* • $Gd_2Re_3Si_5$ *Acta Cryst.* (2014). E**70**, 469–470

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Crystal structure of the ternary silicide $Gd_2Re_3Si_5$

Vitaliia Fedyna, Roksolana Kozak and Roman Gladyshevskii

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Digadolinium trirhenium pentasilicide

Crystal data

$Gd_2Re_3Si_5$
$M_r = 1013.55$
Tetragonal, *P*4/*mnc*
Hall symbol: -P 4 2n
$a = 10.95564$ (13) Å
$c = 5.56326$ (11) Å
$V = 667.74$ (2) Å^3
$Z = 4$
$F(000) = 1692$
$D_x = 10.082$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8564 reflections
$\theta = 1.9$–29.4°
$\mu = 74.55$ mm^{-1}
$T = 293$ K
Irregular, grey
0.16 × 0.10 × 0.02 mm

Data collection

Agilent Xcalibur Onyx diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
CCD scans
Absorption correction: analytical [*CrysAlis PRO* (Agilent, 2012; analytical numeric absorption correction using a multi-faceted crystal model (Clark & Reid, 1995)]
$T_{min} = 0.015$, $T_{max} = 0.194$
11378 measured reflections
502 independent reflections
481 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 29.5°$, $\theta_{min} = 2.6°$
$h = -14 \rightarrow 14$
$k = -15 \rightarrow 14$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.063$
$S = 1.17$
502 reflections
31 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 8.350P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.35$ e Å^{-3}
$\Delta\rho_{min} = -2.44$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00016 (8)

Special details

Experimental. Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by Clark & Reid (1995).

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Gd	0.26249 (5)	0.42271 (5)	0.0000	0.0187 (2)
Re1	0.14676 (4)	0.12315 (4)	0.0000	0.01716 (18)
Re2	0.0000	0.5000	0.2500	0.0173 (2)
Si1	0.0267 (3)	0.3149 (3)	0.0000	0.0192 (6)
Si2	0.17183 (18)	0.67183 (18)	0.2500	0.0145 (6)
Si3	0.0000	0.0000	0.2567 (9)	0.0197 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd	0.0183 (3)	0.0199 (3)	0.0179 (3)	0.0004 (2)	0.000	0.000
Re1	0.0166 (3)	0.0172 (3)	0.0177 (3)	−0.00060 (16)	0.000	0.000
Re2	0.0169 (2)	0.0169 (2)	0.0180 (3)	0.0003 (2)	0.000	0.000
Si1	0.0207 (15)	0.0184 (15)	0.0184 (14)	0.0029 (12)	0.000	0.000
Si2	0.0130 (8)	0.0130 (8)	0.0174 (13)	0.0005 (10)	−0.0025 (8)	0.0025 (8)
Si3	0.0190 (13)	0.0190 (13)	0.021 (2)	0.000	0.000	0.000

Geometric parameters (Å, º)

Gd—Si1	2.841 (4)	Re2—Re2$^{\rm xiv}$	2.7816 (1)
Gd—Si1$^{\rm i}$	2.9604 (12)	Re2—Re2$^{\rm viii}$	2.7816 (1)
Gd—Si1$^{\rm ii}$	2.9604 (12)	Re2—Gd$^{\rm viii}$	3.3047 (5)
Gd—Si3$^{\rm iii}$	3.053 (2)	Re2—Gd$^{\rm xii}$	3.3047 (5)
Gd—Si3$^{\rm iv}$	3.053 (2)	Re2—Gd$^{\rm ii}$	3.3047 (5)
Gd—Re1$^{\rm ii}$	3.1442 (3)	Si1—Re1$^{\rm xi}$	2.467 (4)
Gd—Re1$^{\rm i}$	3.1442 (3)	Si1—Re2$^{\rm viii}$	2.476 (3)
Gd—Si2$^{\rm v}$	3.163 (2)	Si1—Si2$^{\rm viii}$	2.585 (3)
Gd—Si2$^{\rm vi}$	3.163 (2)	Si1—Si2$^{\rm xiii}$	2.585 (3)
Gd—Si2$^{\rm vii}$	3.2202 (11)	Si1—Gd$^{\rm i}$	2.9604 (12)
Gd—Si2	3.2202 (11)	Si1—Gd$^{\rm ii}$	2.9604 (12)
Gd—Re2$^{\rm viii}$	3.3047 (5)	Si2—Re1$^{\rm iii}$	2.4837 (12)
Re1—Si1$^{\rm ix}$	2.467 (4)	Si2—Re1$^{\rm xv}$	2.4837 (12)
Re1—Si1	2.479 (3)	Si2—Si1$^{\rm viii}$	2.585 (3)
Re1—Si2$^{\rm vi}$	2.4838 (12)	Si2—Si1$^{\rm ii}$	2.585 (3)

Re1—Si2^{v}	2.4838 (12)	Si2—Si2^{xvi}	2.7816 (1)
Re1—Si3	2.539 (3)	Si2—Si2^{vii}	2.7816 (1)
Re1—Si3^{x}	2.539 (3)	Si2—Gd^{iii}	3.163 (2)
Re1—Re1^{xi}	2.9683 (6)	Si2—Gd^{xv}	3.163 (2)
Re1—Re1^{ix}	2.9684 (6)	Si2—Gd^{xii}	3.2202 (11)
Re1—Gd^{ii}	3.1442 (3)	Si3—Re1^{x}	2.539 (3)
Re1—Gd^{i}	3.1442 (3)	Si3—Re1^{ix}	2.539 (3)
Re2—Si1^{ii}	2.476 (3)	Si3—Re1^{xi}	2.539 (3)
Re2—Si1^{xii}	2.476 (3)	Si3—Si3^{xvii}	2.707 (9)
Re2—Si1^{viii}	2.476 (3)	Si3—Gd^{ii}	3.053 (2)
Re2—Si1	2.476 (3)	Si3—Gd^{xviii}	3.053 (2)
Re2—Si2^{xiii}	2.662 (3)	Si3—Gd^{xix}	3.053 (2)
Re2—Si2	2.662 (3)	Si3—Gd^{xx}	3.053 (2)

Si1—Gd—Si1^{i}	79.48 (8)	Si1^{ii}—Re2—Gd^{xii}	94.36 (7)
Si1—Gd—Si1^{ii}	79.48 (8)	Si1^{xii}—Re2—Gd^{xii}	56.71 (8)
Si1^{i}—Gd—Si1^{ii}	139.97 (12)	Si1^{viii}—Re2—Gd^{xii}	59.57 (4)
Si1—Gd—Si3^{iii}	152.94 (8)	Si1—Re2—Gd^{xii}	168.30 (6)
Si1^{i}—Gd—Si3^{iii}	127.50 (10)	Si2^{xiii}—Re2—Gd^{xii}	115.730 (10)
Si1^{ii}—Gd—Si3^{iii}	77.03 (10)	Si2—Re2—Gd^{xii}	64.270 (10)
Si1—Gd—Si3^{iv}	152.94 (8)	Re2^{xiv}—Re2—Gd^{xii}	65.111 (4)
Si1^{i}—Gd—Si3^{iv}	77.03 (10)	Re2^{viii}—Re2—Gd^{xii}	114.889 (4)
Si1^{ii}—Gd—Si3^{iv}	127.50 (10)	Gd^{viii}—Re2—Gd^{xii}	74.405 (16)
Si3^{iii}—Gd—Si3^{iv}	52.64 (16)	Si1^{ii}—Re2—Gd^{ii}	56.71 (8)
Si1—Gd—Re1^{ii}	105.17 (3)	Si1^{xii}—Re2—Gd^{ii}	94.36 (7)
Si1^{i}—Gd—Re1^{ii}	172.19 (7)	Si1^{viii}—Re2—Gd^{ii}	168.29 (6)
Si1^{ii}—Gd—Re1^{ii}	47.80 (6)	Si1—Re2—Gd^{ii}	59.57 (4)
Si3^{iii}—Gd—Re1^{ii}	48.34 (7)	Si2^{xiii}—Re2—Gd^{ii}	64.270 (10)
Si3^{iv}—Gd—Re1^{ii}	96.88 (8)	Si2—Re2—Gd^{ii}	115.730 (10)
Si1—Gd—Re1^{i}	105.17 (3)	Re2^{xiv}—Re2—Gd^{ii}	65.111 (4)
Si1^{i}—Gd—Re1^{i}	47.80 (6)	Re2^{viii}—Re2—Gd^{ii}	114.889 (4)
Si1^{ii}—Gd—Re1^{i}	172.19 (7)	Gd^{viii}—Re2—Gd^{ii}	128.540 (19)
Si3^{iii}—Gd—Re1^{i}	96.88 (8)	Gd^{xii}—Re2—Gd^{ii}	130.223 (8)
Si3^{iv}—Gd—Re1^{i}	48.34 (7)	Si1^{ii}—Re2—Gd	59.57 (4)
Re1^{ii}—Gd—Re1^{i}	124.42 (2)	Si1^{xii}—Re2—Gd	168.30 (6)
Si1—Gd—Si2^{v}	81.12 (7)	Si1^{viii}—Re2—Gd	94.36 (7)
Si1^{i}—Gd—Si2^{v}	79.33 (7)	Si1—Re2—Gd	56.71 (8)
Si1^{ii}—Gd—Si2^{v}	129.87 (7)	Si2^{xiii}—Re2—Gd	115.731 (10)
Si3^{iii}—Gd—Si2^{v}	104.01 (5)	Si2—Re2—Gd	64.269 (10)
Si3^{iv}—Gd—Si2^{v}	81.50 (4)	Re2^{xiv}—Re2—Gd	114.888 (4)
Re1^{ii}—Gd—Si2^{v}	95.05 (3)	Re2^{viii}—Re2—Gd	65.112 (4)
Re1^{i}—Gd—Si2^{v}	46.377 (11)	Gd^{viii}—Re2—Gd	130.223 (8)
Si1—Gd—Si2^{vi}	81.12 (7)	Gd^{xii}—Re2—Gd	128.540 (19)
Si1^{i}—Gd—Si2^{vi}	129.87 (7)	Gd^{ii}—Re2—Gd	74.406 (16)
Si1^{ii}—Gd—Si2^{vi}	79.33 (7)	Re1^{xi}—Si1—Re2	122.21 (11)
Si3^{iii}—Gd—Si2^{vi}	81.50 (4)	Re1^{xi}—Si1—Re2^{viii}	122.21 (11)
Si3^{iv}—Gd—Si2^{vi}	104.01 (5)	Re2—Si1—Re2^{viii}	68.34 (9)
Re1^{ii}—Gd—Si2^{vi}	46.377 (11)	Re1^{xi}—Si1—Re1	73.76 (10)

Re1^{i}—Gd—Si2^{vi}	95.05 (3)	Re2—Si1—Re1	139.17 (9)
Si2^{v}—Gd—Si2^{vi}	52.16 (4)	Re2^{viii}—Si1—Re1	139.17 (9)
Si1—Gd—Si2^{vii}	94.12 (8)	Re1^{xi}—Si1—Si2^{viii}	58.84 (9)
Si1^{i}—Gd—Si2^{vii}	49.23 (7)	Re2—Si1—Si2^{viii}	99.03 (11)
Si1^{ii}—Gd—Si2^{vii}	99.13 (6)	Re2^{viii}—Si1—Si2^{viii}	63.42 (8)
Si3^{iii}—Gd—Si2^{vii}	102.67 (6)	Re1—Si1—Si2^{viii}	119.61 (12)
Si3^{iv}—Gd—Si2^{vii}	80.58 (5)	Re1^{xi}—Si1—Si2^{xiii}	58.84 (9)
Re1^{ii}—Gd—Si2^{vii}	135.25 (3)	Re2—Si1—Si2^{xiii}	63.42 (8)
Re1^{i}—Gd—Si2^{vii}	86.902 (11)	Re2^{viii}—Si1—Si2^{xiii}	99.03 (11)
Si2^{v}—Gd—Si2^{vii}	128.074 (8)	Re1—Si1—Si2^{xiii}	119.61 (12)
Si2^{vi}—Gd—Si2^{vii}	175.18 (3)	Si2^{viii}—Si1—Si2^{xiii}	65.09 (9)
Si1—Gd—Si2	94.12 (8)	Re1^{xi}—Si1—Gd	156.27 (14)
Si1^{i}—Gd—Si2	99.13 (6)	Re2—Si1—Gd	76.51 (9)
Si1^{ii}—Gd—Si2	49.23 (7)	Re2^{viii}—Si1—Gd	76.51 (9)
Si3^{iii}—Gd—Si2	80.58 (5)	Re1—Si1—Gd	82.50 (10)
Si3^{iv}—Gd—Si2	102.67 (6)	Si2^{viii}—Si1—Gd	137.86 (11)
Re1^{ii}—Gd—Si2	86.902 (11)	Si2^{xiii}—Si1—Gd	137.86 (11)
Re1^{i}—Gd—Si2	135.25 (3)	Re1^{xi}—Si1—Gd^{i}	84.88 (7)
Si2^{v}—Gd—Si2	175.18 (3)	Re2—Si1—Gd^{i}	141.66 (11)
Si2^{vi}—Gd—Si2	128.075 (8)	Re2^{viii}—Si1—Gd^{i}	74.27 (2)
Si2^{vii}—Gd—Si2	51.18 (2)	Re1—Si1—Gd^{i}	69.99 (6)
Si1—Gd—Re2^{viii}	46.77 (6)	Si2^{viii}—Si1—Gd^{i}	70.63 (3)
Si1^{i}—Gd—Re2^{viii}	46.16 (6)	Si2^{xiii}—Si1—Gd^{i}	132.78 (12)
Si1^{ii}—Gd—Re2^{viii}	95.63 (6)	Gd—Si1—Gd^{i}	87.06 (7)
Si3^{iii}—Gd—Re2^{viii}	149.01 (2)	Re1^{xi}—Si1—Gd^{ii}	84.88 (7)
Si3^{iv}—Gd—Re2^{viii}	118.95 (7)	Re2—Si1—Gd^{ii}	74.27 (2)
Re1^{ii}—Gd—Re2^{viii}	141.358 (16)	Re2^{viii}—Si1—Gd^{ii}	141.66 (11)
Re1^{i}—Gd—Re2^{viii}	92.088 (9)	Re1—Si1—Gd^{ii}	69.99 (6)
Si2^{v}—Gd—Re2^{viii}	103.62 (3)	Si2^{viii}—Si1—Gd^{ii}	132.78 (12)
Si2^{vi}—Gd—Re2^{viii}	127.27 (3)	Si2^{xiii}—Si1—Gd^{ii}	70.63 (3)
Si2^{vii}—Gd—Re2^{viii}	48.14 (5)	Gd—Si1—Gd^{ii}	87.06 (7)
Si2—Gd—Re2^{viii}	72.31 (3)	Gd^{i}—Si1—Gd^{ii}	139.97 (12)
Si1^{ix}—Re1—Si1	163.76 (10)	Re1^{iii}—Si2—Re1^{xv}	131.08 (12)
Si1^{ix}—Re1—Si2^{vi}	62.95 (8)	Re1^{iii}—Si2—Si1^{viii}	170.53 (14)
Si1—Re1—Si2^{vi}	104.06 (9)	Re1^{xv}—Si2—Si1^{viii}	58.21 (7)
Si1^{ix}—Re1—Si2^{v}	62.95 (8)	Re1^{iii}—Si2—Si1^{ii}	58.21 (7)
Si1—Re1—Si2^{v}	104.06 (9)	Re1^{xv}—Si2—Si1^{ii}	170.53 (14)
Si2^{vi}—Re1—Si2^{v}	68.11 (4)	Si1^{viii}—Si2—Si1^{ii}	112.58 (18)
Si1^{ix}—Re1—Si3	96.85 (6)	Re1^{iii}—Si2—Re2	114.46 (6)
Si1—Re1—Si3	96.56 (7)	Re1^{xv}—Si2—Re2	114.46 (6)
Si2^{vi}—Re1—Si3	107.81 (8)	Si1^{viii}—Si2—Re2	56.29 (9)
Si2^{v}—Re1—Si3	159.37 (6)	Si1^{ii}—Si2—Re2	56.29 (9)
Si1^{ix}—Re1—Si3^{x}	96.85 (6)	Re1^{iii}—Si2—Si2^{xvi}	55.947 (19)
Si1—Re1—Si3^{x}	96.56 (7)	Re1^{xv}—Si2—Si2^{xvi}	124.054 (19)
Si2^{vi}—Re1—Si3^{x}	159.37 (6)	Si1^{viii}—Si2—Si2^{xvi}	122.55 (5)
Si2^{v}—Re1—Si3^{x}	107.81 (8)	Si1^{ii}—Si2—Si2^{xvi}	57.45 (5)
Si3—Re1—Si3^{x}	68.46 (18)	Re2—Si2—Si2^{xvi}	90.0
Si1^{ix}—Re1—Re1^{xi}	143.30 (8)	Re1^{iii}—Si2—Si2^{vii}	124.054 (19)

Si1—Re1—Re1^{xi}	52.94 (8)	Re1^{xv}—Si2—Si2^{vii}	55.947 (19)
Si2^{vi}—Re1—Re1^{xi}	141.12 (5)	Si1^{viii}—Si2—Si2^{vii}	57.45 (5)
Si2^{v}—Re1—Re1^{xi}	141.12 (5)	Si1^{ii}—Si2—Si2^{vii}	122.55 (5)
Si3—Re1—Re1^{xi}	54.22 (4)	Re2—Si2—Si2^{vii}	90.0
Si3^{x}—Re1—Re1^{xi}	54.22 (4)	Si2^{xvi}—Si2—Si2^{vii}	180.0
Si1^{ix}—Re1—Re1^{ix}	53.30 (8)	Re1^{iii}—Si2—Gd^{iii}	76.01 (6)
Si1—Re1—Re1^{ix}	142.94 (8)	Re1^{xv}—Si2—Gd^{iii}	66.41 (5)
Si2^{vi}—Re1—Re1^{ix}	106.47 (5)	Si1^{viii}—Si2—Gd^{iii}	112.27 (8)
Si2^{v}—Re1—Re1^{ix}	106.47 (5)	Si1^{ii}—Si2—Gd^{iii}	118.78 (6)
Si3—Re1—Re1^{ix}	54.22 (4)	Re2—Si2—Gd^{iii}	140.83 (3)
Si3^{x}—Re1—Re1^{ix}	54.22 (4)	Si2^{xvi}—Si2—Gd^{iii}	63.919 (19)
Re1^{xi}—Re1—Re1^{ix}	90.0	Si2^{vii}—Si2—Gd^{iii}	116.083 (19)
Si1^{ix}—Re1—Gd^{ii}	116.473 (18)	Re1^{iii}—Si2—Gd^{xv}	66.41 (5)
Si1—Re1—Gd^{ii}	62.214 (12)	Re1^{xv}—Si2—Gd^{xv}	76.01 (6)
Si2^{vi}—Re1—Gd^{ii}	67.22 (4)	Si1^{viii}—Si2—Gd^{xv}	118.78 (6)
Si2^{v}—Re1—Gd^{ii}	127.12 (2)	Si1^{ii}—Si2—Gd^{xv}	112.27 (8)
Si3—Re1—Gd^{ii}	63.95 (8)	Re2—Si2—Gd^{xv}	140.83 (3)
Si3^{x}—Re1—Gd^{ii}	123.79 (8)	Si2^{xvi}—Si2—Gd^{xv}	116.083 (19)
Re1^{xi}—Re1—Gd^{ii}	73.988 (16)	Si2^{vii}—Si2—Gd^{xv}	63.919 (19)
Re1^{ix}—Re1—Gd^{ii}	112.077 (11)	Gd^{iii}—Si2—Gd^{xv}	78.35 (7)
Si1^{ix}—Re1—Gd^{i}	116.473 (18)	Re1^{iii}—Si2—Gd	79.226 (13)
Si1—Re1—Gd^{i}	62.214 (12)	Re1^{xv}—Si2—Gd	120.171 (7)
Si2^{vi}—Re1—Gd^{i}	127.12 (2)	Si1^{viii}—Si2—Gd	94.29 (9)
Si2^{v}—Re1—Gd^{i}	67.22 (4)	Si1^{ii}—Si2—Gd	60.14 (5)
Si3—Re1—Gd^{i}	123.79 (8)	Re2—Si2—Gd	67.59 (5)
Si3^{x}—Re1—Gd^{i}	63.95 (8)	Si2^{xvi}—Si2—Gd	115.588 (10)
Re1^{xi}—Re1—Gd^{i}	73.988 (16)	Si2^{vii}—Si2—Gd	64.411 (10)
Re1^{ix}—Re1—Gd^{i}	112.077 (11)	Gd^{iii}—Si2—Gd	148.88 (7)
Gd^{ii}—Re1—Gd^{i}	124.42 (2)	Gd^{xv}—Si2—Gd	74.63 (2)
Si1^{ix}—Re1—Gd	110.57 (8)	Re1^{iii}—Si2—Gd^{xii}	120.171 (7)
Si1—Re1—Gd	53.19 (8)	Re1^{xv}—Si2—Gd^{xii}	79.226 (13)
Si2^{vi}—Re1—Gd	60.75 (5)	Si1^{viii}—Si2—Gd^{xii}	60.14 (5)
Si2^{v}—Re1—Gd	60.75 (5)	Si1^{ii}—Si2—Gd^{xii}	94.29 (9)
Si3—Re1—Gd	136.39 (6)	Re2—Si2—Gd^{xii}	67.59 (5)
Si3^{x}—Re1—Gd	136.39 (6)	Si2^{xvi}—Si2—Gd^{xii}	64.411 (10)
Re1^{xi}—Re1—Gd	106.13 (2)	Si2^{vii}—Si2—Gd^{xii}	115.588 (10)
Re1^{ix}—Re1—Gd	163.87 (2)	Gd^{iii}—Si2—Gd^{xii}	74.63 (2)
Gd^{ii}—Re1—Gd	73.474 (15)	Gd^{xv}—Si2—Gd^{xii}	148.88 (7)
Gd^{i}—Re1—Gd	73.474 (15)	Gd—Si2—Gd^{xii}	135.19 (9)
Si1^{ii}—Re2—Si1^{xii}	111.66 (9)	Re1—Si3—Re1^{x}	111.54 (18)
Si1^{ii}—Re2—Si1^{viii}	120.57 (15)	Re1—Si3—Re1^{ix}	71.55 (9)
Si1^{xii}—Re2—Si1^{viii}	97.03 (13)	Re1^{x}—Si3—Re1^{ix}	71.55 (9)
Si1^{ii}—Re2—Si1	97.03 (13)	Re1—Si3—Re1^{xi}	71.55 (9)
Si1^{xii}—Re2—Si1	120.57 (15)	Re1^{x}—Si3—Re1^{xi}	71.55 (9)
Si1^{viii}—Re2—Si1	111.66 (9)	Re1^{ix}—Si3—Re1^{xi}	111.54 (18)
Si1^{ii}—Re2—Si2^{xiii}	119.72 (8)	Re1—Si3—Si3^{xvii}	124.23 (9)
Si1^{xii}—Re2—Si2^{xiii}	60.28 (8)	Re1^{x}—Si3—Si3^{xvii}	124.23 (9)
Si1^{viii}—Re2—Si2^{xiii}	119.72 (8)	Re1^{ix}—Si3—Si3^{xvii}	124.23 (9)

Si1—Re2—Si2^{xiii}	60.28 (8)	Re1^{xi}—Si3—Si3^{xvii}	124.23 (9)
Si1^{ii}—Re2—Si2	60.28 (8)	Re1—Si3—Gd^{ii}	67.712 (11)
Si1^{xii}—Re2—Si2	119.72 (8)	Re1^{x}—Si3—Gd^{ii}	151.41 (5)
Si1^{viii}—Re2—Si2	60.28 (8)	Re1^{ix}—Si3—Gd^{ii}	129.93 (3)
Si1—Re2—Si2	119.72 (8)	Re1^{xi}—Si3—Gd^{ii}	81.779 (12)
Si2^{xiii}—Re2—Si2	180.0	Si3^{xvii}—Si3—Gd^{ii}	63.68 (8)
Si1^{ii}—Re2—Re2^{xiv}	55.83 (4)	Re1—Si3—Gd^{xviii}	81.779 (12)
Si1^{xii}—Re2—Re2^{xiv}	55.83 (4)	Re1^{x}—Si3—Gd^{xviii}	129.93 (3)
Si1^{viii}—Re2—Re2^{xiv}	124.17 (4)	Re1^{ix}—Si3—Gd^{xviii}	67.712 (11)
Si1—Re2—Re2^{xiv}	124.17 (4)	Re1^{xi}—Si3—Gd^{xviii}	151.41 (5)
Si2^{xiii}—Re2—Re2^{xiv}	90.0	Si3^{xvii}—Si3—Gd^{xviii}	63.68 (8)
Si2—Re2—Re2^{xiv}	90.0	Gd^{ii}—Si3—Gd^{xviii}	78.66 (6)
Si1^{ii}—Re2—Re2^{viii}	124.17 (4)	Re1—Si3—Gd^{xix}	151.41 (5)
Si1^{xii}—Re2—Re2^{viii}	124.17 (4)	Re1^{x}—Si3—Gd^{xix}	67.712 (11)
Si1^{viii}—Re2—Re2^{viii}	55.83 (4)	Re1^{ix}—Si3—Gd^{xix}	81.779 (12)
Si1—Re2—Re2^{viii}	55.83 (4)	Re1^{xi}—Si3—Gd^{xix}	129.93 (3)
Si2^{xiii}—Re2—Re2^{viii}	90.0	Si3^{xvii}—Si3—Gd^{xix}	63.68 (8)
Si2—Re2—Re2^{viii}	90.0	Gd^{ii}—Si3—Gd^{xix}	127.36 (16)
Re2^{xiv}—Re2—Re2^{viii}	180.0	Gd^{xviii}—Si3—Gd^{xix}	78.66 (6)
Si1^{ii}—Re2—Gd^{viii}	168.29 (6)	Re1—Si3—Gd^{xx}	129.93 (3)
Si1^{xii}—Re2—Gd^{viii}	59.57 (4)	Re1^{x}—Si3—Gd^{xx}	81.779 (12)
Si1^{viii}—Re2—Gd^{viii}	56.71 (8)	Re1^{ix}—Si3—Gd^{xx}	151.41 (5)
Si1—Re2—Gd^{viii}	94.36 (7)	Re1^{xi}—Si3—Gd^{xx}	67.712 (11)
Si2^{xiii}—Re2—Gd^{viii}	64.270 (10)	Si3^{xvii}—Si3—Gd^{xx}	63.68 (8)
Si2—Re2—Gd^{viii}	115.730 (10)	Gd^{ii}—Si3—Gd^{xx}	78.66 (6)
Re2^{xiv}—Re2—Gd^{viii}	114.889 (4)	Gd^{xviii}—Si3—Gd^{xx}	127.36 (16)
Re2^{viii}—Re2—Gd^{viii}	65.111 (4)	Gd^{xix}—Si3—Gd^{xx}	78.66 (6)

Symmetry codes: (i) −*y*+1/2, −*x*+1/2, *z*−1/2; (ii) −*y*+1/2, −*x*+1/2, *z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) *x*+1/2, −*y*+1/2, *z*−1/2; (v) −*y*+1, *x*, −*z*; (vi) −*y*+1, *x*, *z*; (vii) *x*, *y*, −*z*; (viii) −*x*, −*y*+1, −*z*; (ix) *y*, −*x*, −*z*; (x) −*x*, −*y*, −*z*; (xi) −*y*, *x*, *z*; (xii) *y*−1/2, *x*+1/2, −*z*+1/2; (xiii) −*x*, −*y*+1, *z*; (xiv) −*x*, −*y*+1, −*z*+1; (xv) *y*, −*x*+1, −*z*; (xvi) *x*, *y*, −*z*+1; (xvii) −*x*, −*y*, −*z*+1; (xviii) −*x*+1/2, *y*−1/2, −*z*+1/2; (xix) *y*−1/2, *x*−1/2, −*z*+1/2; (xx) *x*−1/2, −*y*+1/2, *z*+1/2.